

Computational study of Mn-doped GaN polar and non-polar surfaces

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ABSTRACT

First-principles calculations were carried out in order to study the magnetic, electronic and structural properties of the Mn-doped polar GaN(0001) and non-polar GaN(10 $\bar{1}$ 0) and GaN(11 $\bar{2}$ 0) surfaces, with the aim of refining the growth of thin films of this material. The results indicate that the surfaces present magnetization of approximately 4.0 μ_B /Mn atom, in agreement with the recently reported theoretical and experimental results. Calculations of surface formation energy indicate that Mn atoms are incorporated into top surface layers (first and second) of GaN, being the Mn_{Ga} incorporation in the polar surface more energetically favourable than in the nonpolar surfaces. In addition, it was observed that the magnetic coupling between the Mn impurities depends on the surface orientation, which could be useful for the design of magnetic nanodevices.

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1. Introduction

Dilute Magnetic Semiconductors (DMS) are semiconductors doped with transition metals atoms in small concentrations; these are placed in substitutional or interstitial positions of the semiconductor [1,2]. The stability at room-temperature of ferromagnetism in DMS could offer excellent opportunities for effective spin manipulation and for the creation of a full spectrum of spintronic devices beyond current technologies. In particular, the manufacture of energy-saving devices, circuits formed by rewritable microchips and low-power magneto resistive random-access memories (MRAM) [3–6]. Among the DMS materials, the Mn-doped GaN systems have been predicted to present a high magnetization and energetic stability, which has recently stimulated the design of electronic nanodevices [7–10]. However, one of the main challenges for spintronic is to synthesize ferromagnetic semiconductors with the Curie temperature (T_c) above room-temperature. Therefore, materials such as gallium nitride (GaN) have been doped with different Mn concentrations and these have shown T_c that could be closer or higher than the room-temperature [11,12]. After that, Dietl et al [13] theoretically predicted a high T_c around 400 K for Mn-doped GaN. A particular interest for understanding the magnetism in this system has increased continuously. For instance, Sasaki et al [14] reported T_c around 940 K for Mn-doped GaN films grown by molecular beam epitaxy. Kronit et al [15] found that

Mn-doped GaN samples could have a half-metallic behaviour, which is promising for spin injection in electronic devices. In addition, the spin lifetime in GaN-based DMS has been predicted to be three orders of magnitude larger than in GaAs-based DMS [16]. On the other hand, theoretical calculations have predicted that the GaN doped with other transition metals could also have a T_c higher than the room-temperature [17–19]. Nevertheless, many recent results on the origin of ferromagnetism in these materials are sometimes contradictory and remain controversial [20,21]. Therefore, in order to refine the growth of magnetic Mn-doped GaN thin films, it is important to understand the Mn incorporation process in the most stable GaN surfaces. In this article, the structural, electronic and magnetic properties of Mn-doped GaN polar (*c*-plane (0001)) and non-polar surfaces (*a*-plane (11 $\bar{2}$ 0) and *m*-plane (10 $\bar{1}$ 0)) are investigated by using first-principle calculations. We explore the source of magnetism and reveal the most stable Mn incorporated configuration in the polar and nonpolar GaN surfaces.

2. Computational methods

All the calculations were performed using the density functional theory (DFT) implemented in the Vienna ab initio simulation package (VASP) [22,23], which performs fully self-consistent calculations to solve the Kohn-Sham equations. Exchange and correlation effects were treated within generalized gradient approximation (GGA) parametrized by the Perdew-Burke-Ernzerhof functional (PBE) [24]. The projector augmented wave method (PAW) was employed to represent core-valence electron

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interactions [25,26], wherein the d states for the Ga and Mn atoms were included as valence electrons. The electronic wavefunctions were expanded as a linear combination of plane waves, and truncated to include only plane waves with kinetic energies less than 500 eV. A Gamma centered grid of $6 \times 6 \times 1$ k-point was used to sample the irreducible Brillouin zone in the Monkhorst-Pack special scheme [27]. Methfessel-Paxton smearing technique with a smearing width of 0.02 Ry was adopted [28]. These parameters ensure a convergence better than 5 meV for the total energy.

GaN polar and nonpolar surfaces were modeled using the supercell approach, where periodic boundary conditions are applied to a central cell so that it is repeated periodically throughout three-dimensional space. An asymmetric slab of 4 GaN bilayers was used for the c -plane (0001) surface and a symmetric slab of 11 and 16 GaN layers was used for the a -plane (11 $\bar{2}$ 0) and m -plane (10 $\bar{1}$ 0) surfaces, respectively. In all the cases, a vacuum region of 16 Å was used in the z direction. In the case of the GaN polar surface, a 2×2 geometry was used and the dangling bonds at the N bottom layer were saturated with pseudo-hydrogen atoms, each with a fractional charge of 0.75 e. The structural optimizations were terminated when the magnitude of the force acting on each ion was less than 1 mRy/Bohr. The magnetic stabilization for the Mn atoms was contrasted by using an initial ferromagnetic (FM) or antiferromagnetic (AFM) spin arrangement for different Mn concentrations. For the electronic band structure calculations, we used the LDA+U method where the Coulomb repulsion energy U and the exchange energy J for Mn atom are chosen to be 4.0 and 0.2 eV respectively [19,20,29,30].

The surface formation energy was calculated from:

$$E_F = E_{total} - E_{ref} - \eta_{Mn}\mu_{(Mn)} - \eta_{Ga}\mu_{(Ga)} - \eta_N\mu_{(N)} \quad (1)$$

where E_{total} is the total energy of the configuration considered, E_{ref} is the total energy of the reference energy (clean GaN polar and non-polar surface), $\mu_{(Mn)}$ is the chemical potential of the atoms of Mn and η_{Mn} is the excess or deficit of atoms of Mn, with respect to the reference the definition is similar for η_{Ga} , η_N , $\mu_{(Ga)}$ y $\mu_{(N)}$ [29–31]. The chemical potentials depend on the experimental conditions under which the material is grown. In order to determine these amounts, we use the relationship: $\mu_{(GaN-bulk)} = \mu_{(Ga)} + \mu_{(N)}$ assuming that the GaN surfaces are in equilibrium with GaN-bulk, where $\mu_{(GaN-bulk)}$ is the chemical potential of GaN in the wurtzite phase. In addition, the chemical potential of each atomic species must be low enough to avoid the formation of undesirable phases [31–33].

Atomic distortion was taken into account by the percentages of change of the layer distances between atomic GaN layers (see Fig. 1) from:

$$\Delta d_{ij} (\%) = \frac{d_{ij} - d_{ij}^0}{d_{ij}^0} \quad (2)$$

where $i = 1, 2, 3, \dots$ and $j = 2, 3, 4, \dots$, d_{ij} are the distances between relaxed atomic layers, d_{ij}^0 are the distances between layers of the surface without relaxing (Fig. 1). The substitution of Ga by Mn is represented by the notation $(z_1/z_2/z_3)$, where z_1 , z_2 and z_3 represent the number of Mn atoms in the first, second and third layers respectively. In Fig. 1, the supercell structures for the GaN nonpolar, a - and m -planes, and the polar, c -plane, are shown, with the substitution of a Ga atom by Mn (Mn_{Ga}) in the first layer, i.e. the (1/0/0) configuration. The a -, m - and c -planes were constructed by means of the stacking of the GaN primitive unit cell in the wurtzite structure with empty regions along the z -axis.

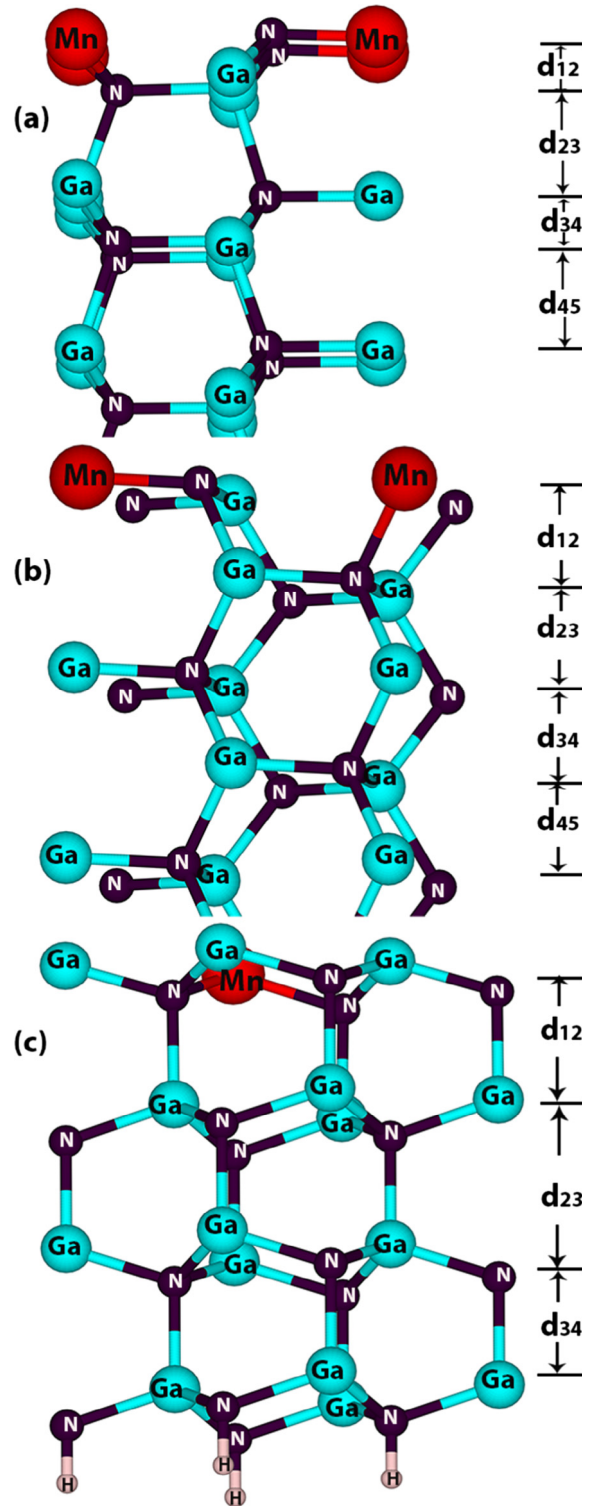


Fig. 1. (1/0/0) configuration for the Mn incorporation on the m -, a - and c -plane GaN, respectively. The d_{12} , d_{23} , d_{34} and d_{45} are the distances between atomic layers.

3. Results and discussion

Gallium nitride bulk calculation was carried out using a wurtzite (hexagonal) unit cell with two lattice parameters a and c , and an internal parameter u . The geometry optimization was performed to vary both the lattice parameters and relaxing the

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